Modeling Rarefied Gas Flows with Direct Simulation Monte Carlo

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Analysis of fluid transport between the continuum and molecular regimes is critical to characterizing and optimizing instruments and vehicles that operate in these conditions. For example, gas transport in microfluidic devices exhibits phenomena that are not present in macroscopic applications. Effects such as rarefaction, thermal creep, and slip boundaries play an important role at microscales and nanoscales and cannot be accurately modeled by continuum solvers due to the molecular nature of the flow.

The degree of noncontinuum behavior is determined by the Knudsen number, the ratio of the mean free path to a characteristic length scale of the flow. Figure 1 depicts the different Knudsen regimes and representative applications. In addition to microfluidic applications, Knudsen number effects are significant in rarefied gas environments and across large gradients such as strong shocks. We intend to implement a direct simulation Monte Carlo (DSMC) capability for subcontinuum fluid flows.

DSMC is a particle-based approach to solving the Boltzmann transport equation. Because the simulated particles are representative of the larger number of gas molecules in the fluid, DSMC is more efficient than purely atomistic simulations like molecular dynamics. Though the original method is applicable to dilute gases, DSMC can be generalized for dense gases with an arbitrary equation of state.

This particle model can be implemented into a computational tool to analyze gas flows in microscale geometries and in larger systems at the dilute limit (high Knudsen number) where the continuum hypothesis is not valid. DSMC has been successfully applied to rarefied and hypersonic flows, but it is also relevant to particle beam focusing, micro-propulsion systems, inertial confinement fusion, and fabrication processes such as vapor deposition and ion etching.

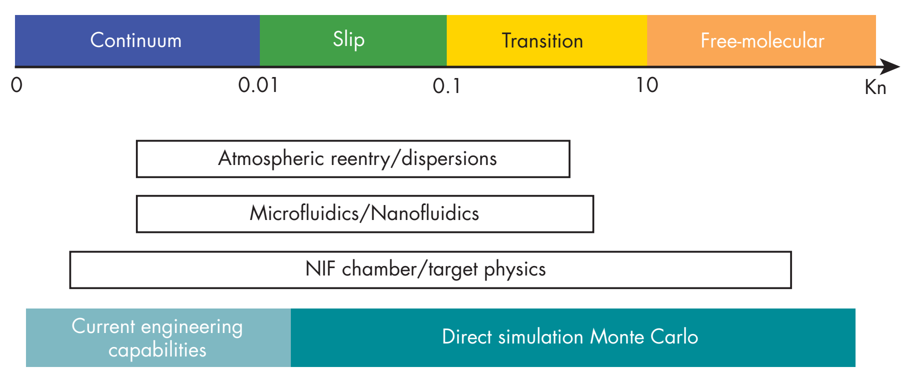

Figure 1. Knudsen number regimes.

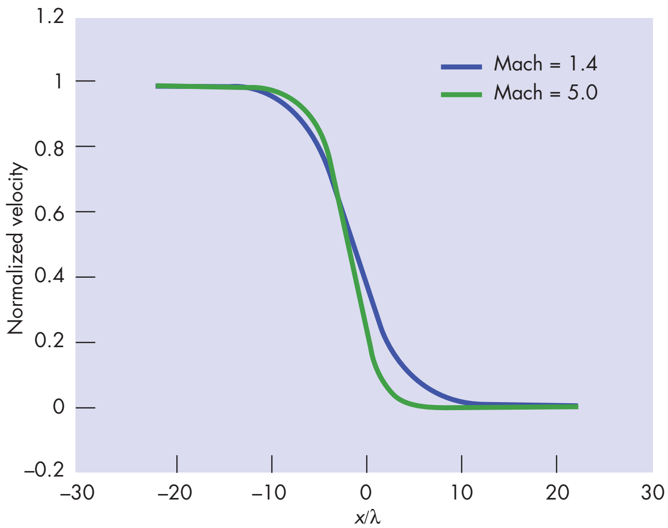

Figure 2. Velocity shock profile for argon gas.

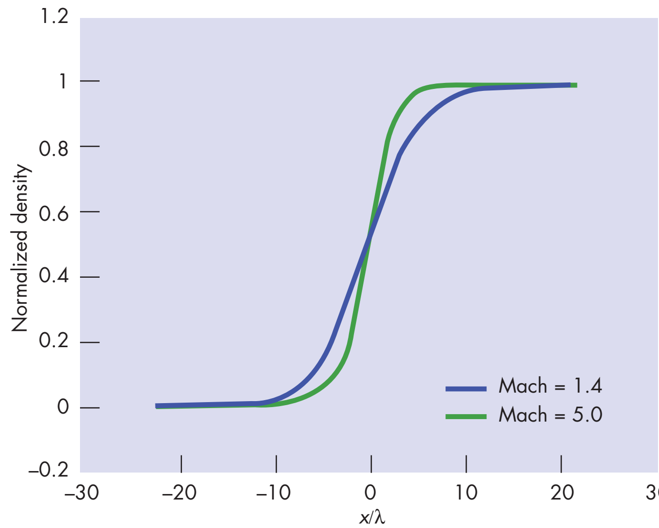

Figure 3. Density shock profile for argon gas.

Project Goals

We will construct a plan for noncontinuum fluid modeling using DSMC methods in the public domain. We will implement these flow solvers and demonstrate this approach for gas flows at both small (microfluidics) and large (hypersonic flight) length scales.

Relevance to LLNL Mission

The implementation of a DSMC algorithm for gas flows will provide LLNL with a new capability relevant to fusion energy and sensors for homeland security. From a scientific perspective, DSMC is an effective tool to investigate nanoscale and noncontinuum physics. A fundamental understanding of phenomena in these regimes will motivate the development of novel devices and systems.

FY2004 Accomplishments and Results

We surveyed potential applications and proven noncontinuum methods. Some of the identified applications for DSMC are indicated in Fig. 1. We also identified published and public domain codes to establish a baseline for features to incorporate into our code. As a basic demonstration of DSMC, we implemented a solver for flow across a stationary shock. Figures 2 and 3 show the shock structure for argon with upstream Mach numbers of 1.4 and 5. The width of the shock is expressed relative to the mean free path.

Related References

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FY2005 Proposed Work

We have proposed to implement and validate a full 3-D DSMC algorithm based on proven methods. We will also extend the capability of the algorithm to dense gases based on a modified Boltzmann approach. Finally, we will provide a demonstration of the code by simulating flow in a microchannel and a jet expansion downstream of a focusing nozzle. As part of our exit strategy, we will explore potential methodologies to couple the particle simulations with continuum solvers and thus provide an interface with other LLNL capabilities.